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ACCURACY OF APPROXIMATE EIGENSTATES

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Abstract

Besides perturbation theory, which requires the knowledge of the exact unperturbed solution, variational techniques represent the main tool for any investigation of the eigenvalue problem of some semibounded operator H in quantum theory. For a reasonable choice of the employed trial subspace of the domain of H, the lowest eigenvalues of H can be located with acceptable precision whereas the trial-subspace vectors corresponding to these eigenvalues approximate, in general, the exact eigenstates of H with much less accuracy. Accordingly, various measures for the accuracy of approximate eigenstates derived by variational techniques are scrutinized. In particular, the matrix elements of the commutator of the operator H and (suitably chosen) different operators with respect to degenerate approximate eigenstates of H obtained by the variational methods are proposed as new criteria for the accuracy of variational eigenstates. These considerations are applied to that Hamiltonian the eigenvalue problem of which defines the spinless Salpeter equation. This bound-state wave equation may be regarded as the most straightforward relativistic generalization of the usual nonrelativistic Schrödinger formalism, and is frequently used to describe, e.g., spin-averaged mass spectra of bound states of quarks.

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1 Motivation

A central element in quantum theory is the solution of eigenvalue problems. However, usually there is no suitable exact solution to which perturbation theory can be applied.

A very efficient way to locate the discrete spectrum of some self-adjoint operator H bounded from below is provided by the famous Rayleigh–Ritz variational technique [1]: *If the eigenvalues E_k, $k = 0, 1, \ldots$, of H are ordered according to $E_0 \leq E_1 \leq E_2 \leq \ldots$, the first d of them are bounded from above by the d eigenvalues $\widehat{E}_k$, $k = 0, 1, \ldots, d-1$, (ordered by $\widehat{E}_0 \leq \widehat{E}_1 \leq \ldots \leq \widehat{E}_{d-1}$) of that operator which is obtained by restricting H to some d-dimensional subspace of the domain of H, i.e., $E_k \leq \widehat{E}_k$, $k = 0, 1, \ldots, d-1$.* Unless the eigenstate $|\chi_k\rangle$ corresponding to some eigenvalue E_k is already an element of this trial space—in which case the upper bound $\widehat{E}_k$ becomes identical to the eigenvalue E_k—, enlarging the dimension d of the trial space will, in general, improve the obtained upper bound; at least, it can't make things worse. However, it is not straightforward to quantify how close approximate eigenstates resulting from the variational method and exact eigenstates are.[1] Thus, we embark upon a systematic study of the accuracy of the variationally determined eigenstates of H and suitable measures to judge their quality.

2 Measures of Quality for Variational Trial States

Consider some self-adjoint operator H, $H^\dagger = H$, assumed to be bounded from below. Suppressing, for the moment, the index $k = 0, 1, 2, \ldots$ discriminating between different solutions, let the eigenvalue equation for H,

$$H|\chi\rangle = E|\chi\rangle \ , \tag{1}$$

be solved by some (generic) eigenvector $|\chi\rangle$ corresponding to some (real) eigenvalue E, to be extracted according to

$$E \equiv \frac{\langle\chi|H|\chi\rangle}{\langle\chi|\chi\rangle} \ .$$

The Rayleigh–Ritz variational technique yields an upper bound $\widehat{E}$ on this eigenvalue E as well as, by diagonalization of the relevant characteristic equation, the corresponding vector $|\varphi\rangle$ in the d-dimensional trial space. There exist several (potentially meaningful) measures of the quality of this trial state $|\varphi\rangle$ which immediately come to one's mind:

1. The trial state $|\varphi\rangle$ is supposed to represent—to a certain degree of accuracy—the approximate solution of the eigenvalue problem defined in Eq. (1). Consequently, a first indicator for the resemblance of $|\varphi\rangle$ with the exact eigenstate $|\chi\rangle$ would be the distance between the expectation value of the operator H with respect to the trial state $|\varphi\rangle$, i.e., between the obtained upper bound

$$\widehat{E} \equiv \frac{\langle\varphi|H|\varphi\rangle}{\langle\varphi|\varphi\rangle} \ ,$$

and the exact eigenvalue E. However, the precise location of the exact eigenvalue E is usually not known. Lower bounds on eigenvalues of self-adjoint operators are much harder to find than upper bounds. The practical use of Temple's inequality [1] is, unfortunately, limited. The "local-energy" theorem [3] applies, in general, only to the ground state.

[1] Recent investigations of the production and decay of heavy quarkonium systems have stimulated renewed interest in the exact value of the wave function at the origin of the two-quark bound state [2].

2. The natural measure for the resemblance of the Hilbert-space vectors $|\varphi\rangle$ and $|\chi\rangle$ under consideration is the overlap

$$S \equiv \frac{\langle\varphi|\chi\rangle}{\sqrt{\langle\varphi|\varphi\rangle\,\langle\chi|\chi\rangle}} \tag{2}$$

of the trial state $|\varphi\rangle$ with the eigenstate $|\chi\rangle$. If the generic eigenstate $|\chi\rangle$ refers to the ground state $|\chi_0\rangle$ of the operator H, the deviation of this overlap from unity is, according to the (rather efficient) Eckart criterion [4], bounded from above by

$$1 - \frac{|\langle\varphi|\chi_0\rangle|^2}{\langle\varphi|\varphi\rangle\,\langle\chi_0|\chi_0\rangle} \leq \frac{1}{E_1 - E_0}\left(\frac{\langle\varphi|H|\varphi\rangle}{\langle\varphi|\varphi\rangle} - E_0\right) \equiv \frac{\widehat{E}_0 - E_0}{E_1 - E_0}\ . \tag{3}$$

A comprehensive discussion of both lower and upper bounds on the overlap S as criteria for the accuracy of approximate wave functions may be found in Ref. [5]. As is evident even from the simple Eckart criterion (3), all these bounds require, in general, some additional knowledge, such as the location of the eigenvalues E_k, $k = 1, 2, \ldots$, of the operator H or matrix elements of higher powers H^n, $n \geq 2$, of H, for instance, certain moments

$$\frac{\langle\varphi|H^n|\varphi\rangle}{\langle\varphi|\varphi\rangle}\ , \quad n \geq 2\ ,$$

of H, or, at least, appropriate bounds on these quantities [5]. Rather frequently, however, the required information is either not available at all or hard to obtain.

3. Consider the commutator $[G, H]$ of the operator H under consideration with any other operator G, where the domain of G is assumed to contain the domain of H. Then the expectation value of this commutator with respect to a given eigenstate $|\chi\rangle$ of H (or, more generally, the matrix element of this commutator with respect to an arbitrary pair of *degenerate* eigenstates $|\chi_i\rangle$ and $|\chi_j\rangle$ of H, i.e., eigenstates which satisfy $E_i = E_j$) trivially vanishes:

$$\langle\chi|[G, H]|\chi\rangle = 0\ . \tag{4}$$

(Under the name "hypervirial theorems" [6], this relation has been generalized, for Hamiltonians H which involve nonrelativistic kinematics, to nonnormalizable vectors $|\chi\rangle$, that is, to vectors which are not elements of some Hilbert space [7].) Hence, choosing different operators G generates a whole class of operators $[G, H]$ each of which may serve to test the quality of a given trial state $|\varphi\rangle$ by evaluating how close the expectation value $\langle\varphi|[G, H]|\varphi\rangle$ of this operator with respect to $|\varphi\rangle$ comes to zero:

$$\langle\varphi|[G, H]|\varphi\rangle \stackrel{?}{\simeq} 0\ .$$

This expectation value vanishes, of course, also if, by accident, the state $|\varphi\rangle$ is an eigenstate of G. However, for a given operator G, after having determined $|\varphi\rangle$, it is straightforward to check for this circumstance, for instance, by inspecting the variance Δ_G of the operator G with respect to the state $|\varphi\rangle$, defined, as usual, by

$$\Delta_G \equiv \frac{\langle\varphi|G^2|\varphi\rangle}{\langle\varphi|\varphi\rangle} - \left(\frac{\langle\varphi|G|\varphi\rangle}{\langle\varphi|\varphi\rangle}\right)^2\ ,$$

which clearly vanishes if the state $|\varphi\rangle$ under consideration is an eigenstate of G. Moreover, it goes without saying that an expectation value $\langle\varphi|[G,H]|\varphi\rangle$ vanishes also if the state $|\varphi\rangle$ is an eigenstate of the commutator $[G,H]$ with eigenvalue 0, or even if the state defined by $[G,H]|\varphi\rangle$ proves to be orthogonal to the state $|\varphi\rangle$.

For any self-adjoint operator G, i.e., $G^\dagger = G$, this commutator is anti-Hermitean, which obviously suggests to define a self-adjoint operator $C = C^\dagger$ (on the domain of the operator H) by

$$[G,H] =: \mathrm{i}\,C \ .$$

If, for example, G is chosen to be the (symmetrized and self-adjoint) generator of dilations,

$$G \equiv \frac{1}{2}\left(\mathbf{x}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{x}\right) \ , \tag{5}$$

the relation (4) is precisely the "master virial theorem" introduced in Ref. [8] for a systematic study of (relativistic) virial theorems [9]. In this case, for operators H of the form of some typical Hamiltonian consisting of a momentum-dependent kinetic-energy operator, $T(\mathbf{p})$, and a coordinate-dependent interaction-potential operator, $V(\mathbf{x})$, that is,

$$H = T(\mathbf{p}) + V(\mathbf{x}) \ ,$$

the operator C becomes the "virial operator"

$$C = \mathbf{p}\cdot\frac{\partial}{\partial\mathbf{p}}T(\mathbf{p}) - \mathbf{x}\cdot\frac{\partial}{\partial\mathbf{x}}V(\mathbf{x}) \ . \tag{6}$$

The point spectrum (i.e., the set of all eigenvalues) of the dilation generator (5) is empty; in other words, the dilation generator has no Hilbert-space eigenvectors.

In any case, however, one should always keep in mind one (trivial) fact [10]: Depending on one's particular choice of the employed trial subspace, it may happen that one trial state $|\varphi^{(1)}\rangle$ yields a better approximation to the exact eigenstate $|\chi\rangle$, as judged by their overlap

$$\frac{\langle\varphi^{(1)}|\chi\rangle}{\sqrt{\langle\varphi^{(1)}|\varphi^{(1)}\rangle\,\langle\chi|\chi\rangle}} \ ,$$

but a worse upper bound $\widehat{E}^{(1)}$ on the corresponding eigenvalue E while some other trial state $|\varphi^{(2)}\rangle$ yields the better upper bound $\widehat{E}^{(2)} < \widehat{E}^{(1)}$ on the eigenvalue E but a worse approximation to the exact eigenstate $|\chi\rangle$, which fact would be betrayed by the overlap

$$\frac{\langle\varphi^{(2)}|\chi\rangle}{\sqrt{\langle\varphi^{(2)}|\varphi^{(2)}\rangle\,\langle\chi|\chi\rangle}} < \frac{\langle\varphi^{(1)}|\chi\rangle}{\sqrt{\langle\varphi^{(1)}|\varphi^{(1)}\rangle\,\langle\chi|\chi\rangle}} \ .$$

3 Prototype of Relativistic Wave Equations: The Spinless Salpeter Equation

Let us apply the above general considerations to the prototype of all (semi-) relativistic bound-state equations, the "spinless Salpeter equation," defined by a—by assumption, self-adjoint—Hamiltonian H (in one-particle form, which encompasses the equal-mass two-particle case, too [11, 12, 13, 14]):

$$H = T + V \ , \tag{7}$$

where T is the "square-root" operator of the relativistic kinetic energy of some particle of mass m and momentum $\mathbf{p}$,

$$T = T(\mathbf{p}) \equiv \sqrt{\mathbf{p}^2 + m^2} \ , \tag{8}$$

and $V = V(\mathbf{x})$ is an arbitrary, coordinate-dependent, static interaction potential. The spinless Salpeter equation is then just the eigenvalue equation for this Hamiltonian H,

$$H|\chi_k\rangle = E_k|\chi_k\rangle \ , \quad k = 0, 1, 2, \dots \ ,$$

for the complete set of Hilbert-space eigenvectors $|\chi_k\rangle$ of H corresponding to its energy eigenvalues

$$E_k \equiv \frac{\langle\chi_k|H|\chi_k\rangle}{\langle\chi_k|\chi_k\rangle} \ .$$

Analytic upper bounds on these eigenvalues have been given [11, 12, 13, 14, 15, 16, 17]. For the Coulomb potential, the local-energy theorem has been successfully applied [18].

For the sake of comparison, we focus our interest to central potentials $V(\mathbf{x}) = V(r)$, $r \equiv |\mathbf{x}|$. Furthermore, in order to facilitate the numerical treatment of the problem, we consider the harmonic-oscillator potential

$$V(r) = a\, r^2 \ , \quad a > 0 \ . \tag{9}$$

The reason for this particular choice is the following: In momentum space, the operator r^2 is represented by the Laplacian with respect to the momentum $\mathbf{p}$, $r^2 \to -\Delta_{\mathbf{p}}$, while the kinetic energy T, nonlocal in configuration space, is represented by a multiplication operator. Consequently, exactly for a harmonic-oscillator potential the semirelativistic Hamiltonian H in its momentum-space representation is equivalent to a nonrelativistic Hamiltonian with some (effective) interaction potential reminiscent of the square root:

$$H = -a\, \Delta_{\mathbf{p}} + \sqrt{\mathbf{p}^2 + m^2} \ . \tag{10}$$

The solutions of the corresponding eigenvalue equation may then be found with one of the numerous procedures designed for the treatment of the nonrelativistic Schrödinger equation.

For the harmonic-oscillator potential, it is comparatively easy to get a first idea of the approximate location of the energy levels E_k by entirely analytical considerations:

- On the one hand, since

  $$T(\mathbf{p}) \leq m + \frac{\mathbf{p}^2}{2\,m} \ ,$$

  every energy eigenvalue E_k of H is bounded from above by the energy eigenvalue $E_{k,\mathrm{NR}}$ of the nonrelativistic counterpart

  $$H_{\mathrm{NR}} = m + \frac{\mathbf{p}^2}{2\,m} + V$$

  of H:

  $$E_k \leq E_{k,\mathrm{NR}} \ .$$

  For the harmonic-oscillator potential (9), these nonrelativistic energy levels read

  $$E_{\mathrm{NR}} = m + \sqrt{\frac{2\,a}{m}}\, \left(2\, n_{\mathrm{r}} + \ell + \frac{3}{2}\right) , \tag{11}$$

  expressed in terms of radial quantum number $n_{\mathrm{r}} = 0, 1, 2, \dots$ and orbital angular momentum $\ell = 0, 1, 2, \dots$. An (easily) improved bound may be found in App. A.

- On the other hand, since
$$T(\mathbf{p}) \geq |\mathbf{p}| \ ,$$
every energy eigenvalue E_k of H is bounded from below by the energy eigenvalue $E_k(m=0)$ of the Hamiltonian
$$H(m=0) = |\mathbf{p}| + V$$
corresponding to vanishing particle mass m:
$$E_k \geq E_k(m=0) \ .$$
For the harmonic-oscillator potential (9), by remembering the momentum-space representation (10) of H all bound states of vanishing orbital angular momentum ℓ ("S waves") may be obtained as solutions of a differential equation of the form
$$\frac{\mathrm{d}^2}{\mathrm{d}z^2} f(z) - z\, f(z) = 0 \ ;$$
the resulting energy levels read
$$E(m=0) = -a^{1/3}\, z_0 \ ,$$
where z_0 denote the zeros of the Airy function $\mathrm{Ai}(z)$, which solves this differential equation: $z_0 = -2.33810\ldots, -4.08794\ldots, -5.52055\ldots, \ldots$ [19]. Energy levels of bound states of nonvanishing orbital angular momentum ℓ ("P, D, ... waves") must be determined numerically anyway. Also this bound is improved in App. A.

For homogeneous functions, the radial derivatives entering in the virial operator (6) simply probe the respective degree of homogeneity of these functions. In particular, for the harmonic-oscillator potential (9) one finds
$$\mathbf{x} \cdot \frac{\partial}{\partial \mathbf{x}} V(\mathbf{x}) = r\, \frac{\partial}{\partial r} V(r) = 2\, a\, r^2 = 2\, V(r) \ .$$
With the expression (6) for C, introducing the (only momentum-dependent) operator
$$F \equiv T(\mathbf{p}) + \frac{1}{2}\, \mathbf{p} \cdot \frac{\partial}{\partial \mathbf{p}} T(\mathbf{p}) \ ,$$
the Hamiltonian (7) with harmonic-oscillator potential thus may be cast into the form
$$\begin{aligned} H &= T(\mathbf{p}) + V(\mathbf{x}) \\ &= T(\mathbf{p}) + \frac{1}{2}\, \mathbf{x} \cdot \frac{\partial}{\partial \mathbf{x}} V(\mathbf{x}) \\ &= T(\mathbf{p}) + \frac{1}{2}\, \mathbf{p} \cdot \frac{\partial}{\partial \mathbf{p}} T(\mathbf{p}) - \frac{C}{2} \\ &\equiv F - \frac{C}{2} \ . \end{aligned}$$
This observation allows to express any matrix element of the operator C (in particular, its expectation value $\langle\varphi|C|\varphi\rangle$ with respect to the trial state $|\varphi\rangle$ under investigation) as the corresponding matrix element of the difference of Hamiltonian H and operator F:
$$\langle\varphi|C|\varphi\rangle = 2\, \langle\varphi|F - H|\varphi\rangle \equiv 2\, \Big(\langle\varphi|F|\varphi\rangle - \widehat{E}\, \langle\varphi|\varphi\rangle \Big) \, .$$
For the relativistic expression (8) of the kinetic energy T, the above operator F reads
$$F = \frac{3\, \mathbf{p}^2 + 2\, m^2}{2\, \sqrt{\mathbf{p}^2 + m^2}} \ .$$

4 Definition of the "Laguerre" Trial Space

As far as the achieved accuracy of the solutions obtained is concerned, the most crucial step in all variational games of the Rayleigh–Ritz kind is, for a given operator H under consideration, a reasonable definition of the adopted trial subspace of the domain of H.

For spherically symmetric potentials $V(r)$, a very popular choice for the basis states which span the trial space required for the application of the variational technique are "Laguerre" trial states, given in configuration-space representation by [20, 16, 13, 14]

$$\psi_{k,\ell m}(\mathbf{x}) = \sqrt{\frac{(2\,\mu)^{2\,\ell+2\,\beta+1}\,k!}{\Gamma(2\,\ell+2\,\beta+k+1)}}\,r^{\ell+\beta-1}\exp(-\mu\,r)\,L_k^{(2\,\ell+2\,\beta)}(2\,\mu\,r)\,\mathcal{Y}_{\ell m}(\Omega_{\mathbf{x}})\ , \qquad (12)$$

where $L_k^{(\gamma)}(x)$ are the generalized Laguerre polynomials (for parameter γ) [19], defined by the power series

$$L_k^{(\gamma)}(x) = \sum_{t=0}^{k}(-1)^t \left(\begin{array}{c} k+\gamma \\ k-t \end{array} \right) \frac{x^t}{t!}$$

and normalized, with the weight function $x^\gamma \exp(-x)$, according to

$$\int\limits_0^\infty \mathrm{d}x\,x^\gamma \exp(-x)\,L_k^{(\gamma)}(x)\,L_{k'}^{(\gamma)}(x) = \frac{\Gamma(\gamma+k+1)}{k!}\,\delta_{kk'}\ ,$$

and $\mathcal{Y}_{\ell m}(\Omega)$ are the spherical harmonics for angular momentum ℓ and its projection m, depending on the solid angle Ω and orthonormalized according to

$$\int \mathrm{d}\Omega\,\mathcal{Y}^*_{\ell m}(\Omega)\,\mathcal{Y}_{\ell' m'}(\Omega) = \delta_{\ell\ell'}\,\delta_{mm'}\ .$$

The trial functions (12) involve two variational parameters, μ (with dimension of mass) and β (dimensionless), which, by the requirement of normalizability of these functions, are subject to the constraints $\mu > 0$ and $2\,\beta > -1$.

One of the advantages of the trial function (12) is the easy availability of an analytic expression for the corresponding momentum-space representation of these trial states, obtained by Fourier transformation:

$$\begin{aligned}
\widetilde{\psi}_{k,\ell m}(\mathbf{p}) \;&=\; \sqrt{\frac{(2\,\mu)^{2\,\ell+2\,\beta+1}\,k!}{\Gamma(2\,\ell+2\,\beta+k+1)}}\,\frac{(-\mathrm{i})^\ell\,|\mathbf{p}|^\ell}{2^{\ell+1/2}\,\Gamma\left(\ell+\frac{3}{2}\right)}\sum_{t=0}^{k}\frac{(-1)^t}{t!}\left(\begin{array}{c} k+2\,\ell+2\,\beta \\ k-t \end{array} \right) \\
&\times\; \frac{\Gamma(2\,\ell+\beta+t+2)\,(2\,\mu)^t}{(\mathbf{p}^2+\mu^2)^{(2\,\ell+\beta+t+2)/2}}\,F\left(\frac{2\,\ell+\beta+t+2}{2},-\frac{\beta+t}{2};\ell+\frac{3}{2};\frac{\mathbf{p}^2}{\mathbf{p}^2+\mu^2}\right) \\
&\times\; \mathcal{Y}_{\ell m}(\Omega_{\mathbf{p}})\ ,
\end{aligned}$$

with the hypergeometric series F, defined by

$$F(u,v;w;z) = \frac{\Gamma(w)}{\Gamma(u)\,\Gamma(v)}\sum_{n=0}^{\infty}\frac{\Gamma(u+n)\,\Gamma(v+n)}{\Gamma(w+n)}\,\frac{z^n}{n!}\ .$$

For the present investigation, we too employ the "Laguerre" trial states defined by Eq. (12), with, for both definiteness and ease of calculation, the variational parameters μ and β kept fixed to the values $\mu = m$ and $\beta = 1$.[2]

[2] Within some specific nonrelativistic quark potential model, the significance of the wave function at the origin obtained variationally from superpositions of Gaussian trial functions has been discussed numerically [21].

Of course, the trivial fact that the (Hilbert-space) states defined by the "Laguerre" trial functions (12) cannot be eigenvectors of the dilation generator (5) is reflected by the nonvanishing numerical value of the variance Δ_G of the operator G in these states: For instance, for the lowest-dimensional possibility, $d = 1$, realized by the trial function

$$\psi_{0,00}(\mathbf{x}) = \sqrt{\frac{\mu^3}{\pi}} \exp(-\mu\, r) \ ,$$

this variance is exactly $\Delta_G = 3/4$. For trial-space dimension $d = 25$, this quantity takes in the state corresponding to the lowest eigenvalue $\widehat{E}$ the numerical value $\Delta_G = 1.3779$.

Up to a dimension $d = 4$ of the trial space, the matrix elements of the Hamiltonian H with respect to the chosen trial states are, at least in principle, accessible by entirely algebraic manipulations. In the simplest conceivable case, realized by the choice $d = 1$, one finds with the help of the explicit analytic expressions for the matrix elements of H derived in Ref. [16], for instance, for the ground-state energy E_0 the naive upper bound

$$\widehat{E}_0 = \frac{64\, m}{15\, \pi} + \frac{3\, a}{m^2} \ .$$

5 Rates of Convergence of the Quality Measures

Now, let us observe our variational eigenstates, $|\varphi\rangle$, approaching the exact eigenstates, $|\chi\rangle$, for increasing dimension d of the employed trial space, by comparing the behaviour of the various measures for the accuracy of approximate eigenstates discussed in Sec. 2.

Without doubt, the only genuine "point of reference" of any variational solution to an eigenvalue problem is the corresponding exact solution. The exact solution sought is computed here with the help of the numerical integration procedure developed for the solution of the nonrelativistic Schrödinger equation in Ref. [22]. (Since the problematic term in our Hamiltonian is the kinetic-energy operator (8), the solution is constructed in momentum space,[3] which, in addition, allows to take advantage of the operator F.)

Table 1 confronts, for the ground state and the lowest radial and orbital excitations, the approximate solutions as calculated with the help of the Rayleigh–Ritz variational technique for "Laguerre" trial subspaces of the domain of H of increasing dimension d with the exact solutions of the eigenvalue problem for the semirelativistic Hamiltonian (7) with a central interaction potential of the harmonic-oscillator form (9). First of all, as discussed in Sec. 3, the exact position of any eigenvalue E of our Hamiltonian H is confined to a range defined by the nonrelativistic upper bound E_{NR} and the zero-mass lower bound $E(m = 0)$ on this energy eigenvalue E. There are several quantities which may participate in a competition for "the best or most reasonable measure of quality:"

1. The relative error ε of every (Rayleigh–Ritz) upper bound $\widehat{E}$ on the exact energy eigenvalue E,

$$\varepsilon \equiv \frac{\widehat{E} - E}{E} \ , \tag{13}$$

is, by definition, always nonnegative, i.e.,

$$\varepsilon \geq 0 \ .$$

[3] The outcome of any numerical integration procedure is a solution given only at discrete points in the respective representation space. The reconstruction of the entire function, with the help of some interpolation procedure, in form of an interpolating function introduces, clearly, an additional error. We have, of course, checked that this error is negligible.

Table 1: Characterization of the quality of the variational solution of the eigenvalue problem of the semirelativistic Hamiltonian $H = \sqrt{\mathbf{p}^2 + m^2} + V(r)$ with harmonic-oscillator potential $V(r) = a\, r^2$, for states of radial quantum number $n_\mathrm{r} = 0, 1, 2$ and orbital angular momentum $\ell = 0, 1, 2$ (called 1S, 2S, 3S, 1P, and 1D in usual spectroscopic notation), obtained with the help of "Laguerre" trial states spanning trial spaces of increasing dimension $d = 1, 2, 3, 10, 25$, by: the nonrelativistic upper bound E_NR and zero-mass lower bound $E(m = 0)$ on the energy, the (numerically computed) "exact" energy E, the variational upper bound $\widehat{E}$ on this energy, the relative error ε of the upper bound, the deviation from unity, σ, of the overlap squared of exact and variational eigenstates, the (appropriately normalized) expectation values ν of the virial operator C, and the (normalized) maximum local difference ω of the momentum-space representations of exact and variational eigenstates. The physical parameters are fixed to the values $m = 2$ GeV for the particle mass and $a = 2$ GeV^3 for the harmonic-oscillator coupling. A simple entry "0" indicates that the numerical value is closer to 0 than the rounding error.

Quantity	d	State				
		1S	2S	3S	1P	1D
n_r		0	1	2	0	0
ℓ		0	0	0	1	2
E_NR [GeV]		4.12132	6.94975	9.77817	5.53553	6.94975
$E(m = 0)$ [GeV]		2.94583	5.15049	6.95547	4.23492	5.35237
E [GeV]		3.82493	5.79102	7.48208	4.90145	5.89675
$\widehat{E}$ [GeV]	1	4.21624	—	—	6.50936	9.77866
	2	3.92759	8.10850	—	5.24154	7.18242
	3	3.92684	6.40425	14.4358	4.98863	6.32228
	10	3.82530	5.82005	7.64092	4.90409	5.90122
	25	3.82494	5.79114	7.48290	4.90149	5.89681
ε [cf. Eq. (13)]	1	0.1023	—	—	0.3280	0.6583
	2	0.0268	0.4002	—	0.0694	0.2180
	3	0.0266	0.1059	0.9294	0.0178	0.0722
	10	0.0001	0.0050	0.0212	0.0005	0.0008
	25	0	0	0.0001	0	0
σ [cf. Eq. (14)]	1	0.09618	—	—	0.36144	0.65587
	2	0.02375	0.43693	—	0.09001	0.34398
	3	0.02280	0.13878	0.83034	0.01918	0.12705
	10	0.00003	0.00560	0.03727	0.00040	0.00061
	25	0	0	0.00008	0	0
ν [cf. Eq. (15)]	1	−0.6120	—	—	−0.8328	−0.9074
	2	+0.0308	−0.8666	—	−0.5103	−0.7483
	3	−0.0187	−0.4577	−0.9525	−0.1275	−0.5197
	10	−0.0034	−0.0167	−0.1895	−0.0016	−0.0175
	25	0	−0.0001	+0.0001	0	0
ω [cf. Eq. (16)]	1	+0.9277	—	—	+0.7541	+1.0578
	2	−0.00754	+2.4577	—	+0.3598	+0.7262
	3	−0.01049	+0.2265	+4.3252	+0.1146	+0.4209
	10	−0.00867	+0.0587	+0.2592	+0.0183	+0.0186
	25	+0.00003	−0.0017	+0.0002	+0.0004	+0.0003

2. The deviation from unity, σ, of the modulus squared of the overlap S of exact and variational eigenstates defined in Eq. (2),

$$\sigma \equiv 1 - |S|^2 \ , \tag{14}$$

is clearly confined to the range

$$0 \leq \sigma \leq 1 \ ;$$

the lower bound applies when the variational eigenstate $|\varphi\rangle$ *agrees* with the exact eigenstate $|\chi\rangle$, while the upper bound applies when the variational eigenstate $|\varphi\rangle$ is *orthogonal* to the exact eigenstate $|\chi\rangle$. Just for comparison, the Eckart bounds (3) on σ, unfortunately available only for the ground state, are given in Table 2. In our case, these bounds turn out to be always larger than the actual numerical values of the ground-state overlap by at least a factor 2.

Table 2: Eckart bounds on the difference to unity of the overlap squared σ of Eq. (14) (which apply only to the ground state, identified by vanishing radial and orbital-angular-momentum quantum numbers $n_{\rm r} = \ell = 0$) for increasing dimension $d = 1, 2, 3, 10, 25$ of the trial subspace

d	$\frac{\widehat{E}_0 - E_0}{E_1 - E_0}$
1	0.19903
2	0.05222
3	0.05183
10	0.00019
25	0.00001

3. The use of the expectation values of the commutators $[G, H]$ with respect to the variational eigenstates $|\varphi\rangle$ is illustrated for the particular example of the dilation generator G defined in Eq. (5), by considering (suitably normalized) expectation values $\langle\varphi|C|\varphi\rangle$ of the virial operator C given in Eq. (6):

$$\nu \equiv \frac{\langle\varphi|C|\varphi\rangle}{\langle\varphi|\mathbf{x}\cdot\frac{\partial}{\partial\mathbf{x}}V(\mathbf{x})|\varphi\rangle} = \frac{\langle\varphi|\mathbf{p}\cdot\frac{\partial}{\partial\mathbf{p}}T(\mathbf{p})|\varphi\rangle}{\langle\varphi|\mathbf{x}\cdot\frac{\partial}{\partial\mathbf{x}}V(\mathbf{x})|\varphi\rangle} - 1 \ . \tag{15}$$

4. Finally, the normalized maximum difference of the normalized momentum-space representations $\tilde{\varphi}(\mathbf{p})$ and $\tilde{\chi}(\mathbf{p})$ of variational eigenstate $|\varphi\rangle$ and exact eigenstate $|\chi\rangle$, respectively, i.e., the maximum pointwise relative error in momentum space,

$$\omega \equiv \frac{\max\limits_{\mathbf{p}}[\tilde{\varphi}(\mathbf{p}) - \tilde{\chi}(\mathbf{p})]}{\max\limits_{\mathbf{p}}\tilde{\chi}(\mathbf{p})} \tag{16}$$

is listed.

Note that the only measure for the accuracy of approximate eigenstates $|\varphi\rangle$ which does not require any information other than the one provided by the variational technique is ν, the (normalized) expectation values of the commutator $[G, H]$ with respect to $|\varphi\rangle$. Inspection of Table 1 reveals that ν represents indeed a sensitive measure of quality: for increasing trial-space dimension d it converges to zero at roughly the same rate as both energy and overlap error, ε and σ, but makes more sense than a pointwise error like ω.

6 Summary and Conclusions

This work has been devoted to a systematic investigation of the quality of solutions of the eigenvalue problem for some (semibounded, self-adjoint) operator H by variational methods. Clearly, even if the overlap of a variationally derived approximate eigenstate and the corresponding exact eigenstate is close to unity, this does not necessarily imply that expectation values of given operators (among which this operator H which defines the particular eigenvalue problem under consideration is just one) with respect to these two eigenstates are equal to the same degree of accuracy. For instance, a given operator might probe regions in representation space where the difference between approximate and exact solutions is of less importance for the overlap. (Only for functions $f(H)$ of H, the difference between approximate and exact expectation values of f is, in general, of second order in the deviation of the approximate eigenstate from the exact eigenstate.) In view of this, various measures for the accuracy of approximate eigenstates have been discussed. Apart from the possible exception of some more or less pathological special cases (cf. our corresponding remarks in Sec. 2), the vanishing of the expectation values of the commutator of H and any other well-defined operator, taken with respect to the approximate eigenstates, provides a useful set of criteria for estimating the significance of the variational solution. This has been illustrated by considering the commutator of the Hamiltonian of the spinless Salpeter equation—which represents the first step from the nonrelativistic Schrödinger formalism towards incorporation of relativistic effects and which is used for the semirelativistic description of the spin-averaged mass spectra of bound states of "constituent" quarks within the framework of potential models (for analyses of these attempts see, e.g., Refs. [23, 24, 25])—and the generator of dilations.

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A The Relativistic Harmonic-Oscillator Problem

In spite of the fact that it is somewhat off the main stream of the present investigation, let us demonstrate how, with only slightly more effort, the bounds on the energy levels of the relativistic harmonic oscillator derived in Sec. 3 may be considerably improved:[4]

- By considering the square of the (obviously self-adjoint) operator $T-\mu$, where μ is an arbitrary real parameter (with the dimension of mass), one obtains a set of operator inequalities for the kinetic energy T given in Eq. (8) [26, 12, 13, 14, 17]:

$$T \leq \frac{\mathbf{p}^2 + m^2 + \mu^2}{2\,\mu} \quad \text{for all } \mu > 0 \ .$$

  These inequalities immediately translate into upper bounds on the energy levels E_k, $k = 0, 1, 2, \ldots$, of the relativistic harmonic-oscillator problem, which involve the corresponding nonrelativistic energy eigenvalues $E_{k,\mathrm{NR}}$ recalled in Eq. (11):

$$E_k \leq E_{k,\mathrm{upper}}(\mu) \equiv \frac{m^2 + \mu^2}{2\,\mu} + \sqrt{\frac{m}{\mu}}\,(E_{k,\mathrm{NR}} - m)\,, \quad \mu > 0 \ .$$

[4] We thank the referee, presumably André Martin, for his "suggestion" to include this discussion.

- On the other hand, by taking into account, for instance, the obvious positivity of the square of the (self-adjoint) operator $\mathbf{p}^2\,\xi^2 - m^2\,(1-\xi^2)$ for an arbitrary real parameter ξ, it is straightforward to convince oneself of the validity of the set of operator inequalities

$$T \geq |\mathbf{p}|\,\sqrt{1-\xi^2} + m\,\xi \ , \quad 0 \leq \xi \leq 1 \ .$$

  Remembering the energy eigenvalues $E_k(m=0)$ of the Hamiltonian $H(m=0)$ corresponding to vanishing particle mass m introduced in Sec. 3, these operator inequalities may be reformulated in a straightforward way as lower bounds on the energy levels E_k, $k = 0, 1, 2, \ldots$, of the relativistic harmonic-oscillator problem:

$$E_k \geq E_{k,\mathrm{lower}}(\xi) \equiv \xi\,m + (1-\xi^2)^{1/3}\,E_k(m=0) \ , \quad 0 \leq \xi \leq 1 \ .$$

Numerical optimization of these bounds with respect to the parameters μ and ξ then yields the improved upper and lower bounds on the energies of the lowest-lying states of the relativistic harmonic oscillator listed in Table 3.

Table 3: Improved upper and lower bounds on the lowest energy levels of the semirelativistic Hamiltonian $H = \sqrt{\mathbf{p}^2 + m^2} + V(r)$ with harmonic-oscillator potential $V(r) = a\,r^2$, for states with radial quantum number $n_\mathrm{r} = 0, 1, 2$ and orbital angular momentum $\ell = 0, 1, 2$ (denoted by 1S, 2S, 3S, 1P, and 1D in usual spectroscopic notation), for a particle mass of $m = 2$ GeV and a harmonic-oscillator coupling strength of $a = 2$ GeV^3.

Optimized Bounds	State				
	1S	2S	3S	1P	1D
n_r	0	1	2	0	0
ℓ	0	0	0	1	2
$\min\limits_{\mu} E_{\mathrm{upper}}(\mu)$ [GeV]	3.89851	5.99081	7.80385	4.98990	5.99081
$\max\limits_{\xi} E_{\mathrm{lower}}(\xi)$ [GeV]	3.75534	5.68007	7.36329	4.85577	5.86508

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